Synthetic, Crystallographic, and Computational Study of Copper(II) Complexes of Ethylenediaminetetracarboxylate Ligands

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Supporting Information Available: CCDC 891689 contain the supplementary crystallographic data. These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk. Structural data for Ba[Cu(eda3p)]·8H_2O considered herein (Table S1), conformations of *N*-membered rings (Table S2) and data of IR spectra of Cu-edta-type of complexes (Table S3).

Table S1. Structural data for $Ba[Cu(eda3p)]\cdot 8H_2O$

M-L bond lengths (Å)			
Cu-O1	1.9514(17)		
Cu-O3	2.5180(17)		
Cu-O5	2.2994(16)		
Cu-O7	2.0130(16)		
Cu-N1	2.026(2)		
Cu-N2	2.022(2)		
M-O-C angles (°)			
Cu-O1-C1	128.12(16)		
Cu-O3-C6	100.24(15)		
Cu-O7-C13	113.05(14)		
Cu-O5-C11	108.27(15)		
Bond angles (°)			
Cis angles		*Trans* angles	
O3-Cu-O7	79.26(6)	O1-Cu-N2	174.67(8)
O3-Cu-N1	86.80(7)	O3-Cu-O5	166.68(5)
O3-Cu-N2	95.42(7)	O7-Cu-N1	162.46(9)
O5-Cu-O7	89.38(6)		
O5-Cu-N1	105.59(7)		
O5-Cu-N2	89.88(7)		
O7-Cu-N2	82.32(7)		
N1-Cu-N2	88.51(9)		
O7-Cu-O1	97.11(7)		
O3-Cu-O1	89.66(6)		
O5-Cu-O1	84.82(7)		
O1-Cu-N1	93.37(9)		

Table S2. Conformations of *N*-membered Rings ($N \leq 8$)

Ring Size *N*	Definition	Descriptive Name	Descriptive Symbol
4	$q_2 \neq 0$	puckered form	
5	$q_2 > 0;\ \phi_2 = 0$	envelope	
	$q_2 > 0;\ \phi_2 = \pi/2$	twist form	
6	$q_3 = 0;\ q_2 > 0;\ \phi_2 = 0$	boat	
	$q_3 = 0;\ q_2 > 0;\ \phi_2 = \pi/2$	twist-boat	
	$q_2 = 0;\ q_3 \neq 0$	chair	
7	$q_3 = 0;\ q_2 > 0;\ \phi_2 = 0$	boat	
	$q_3 = 0;\ q_2 > 0;\ \phi_2 = \pi/2$	twist-boat	
	$q_2 = 0;\ q_3 > 0;\ \phi_3 = 0$	chair	
	$q_2 = 0;\ q_3 > 0;\ \phi_3 = \pi/2$	twist-chair	
8	$q_4 = q_3 = 0;\ q_2 > 0;\ \phi_2 = 0$	boat-boat	
	$q_4 = q_3 = 0;\ q_2 > 0;\ \phi_2 = \pi/2$	twist-boat	
	$q_4 = q_2 = 0;\ q_3 > 0;\ \phi_3 = 0$	long-chair	
	$q_4 = q_2 = 0;\ q_3 > 0;\ \phi_3 = \pi/2$	twist-chair	
	$q_3 = q_2 = 0;\ q_4 \neq 0$	crown	

Table S3. Data of IR spectra of Cu-edta-type of complexes

Complex	Vibration (cm^{-1}) ν_{asym} (COOM)	Chelate ring sze	Reference
trans(O5)-[BaCu(edta)(H_2O)$_3$]·H_2O	1600	5	*
trans(O5)-Mg[Cu(ed3ap)]·8H_2O	1683	5	This work
	1598	6	
trans(O5)- Ba[Cu(eddadp)]·8H_2O	1598	5 and 6	This work
trans(O6)-Ba[Cu(eda3p)]·8H_2O	1575	6	This work
	1623	5	
[Mg(H_2O)$_5$][Cu(edtp)]	1572	6	(35)

*Insausti, M.; Pizarro, J. L.; Lezama, L., Cortes, R.; Bocanegra, E. H.; Arriortua, M. I.; Rojo, T. *Chem. Mater.* **1994**, *6*, 707-713.